

## A North American Fibre Diffraction Network

A number of fibre diffraction laboratories in the USA have joined together to form an American network that will be similar to CCP13 in many of its goals and activities, and will work closely with CCP13 for the development of fibre diffraction on both sides of the Atlantic. The network, formally known as Research Coordination Network: Fiber Diffraction from Biological Polymers and Assemblies, and informally as *FiberNet*, is supported by the US National Science Foundation.

The goal of the network is to develop biological fibre diffraction methods, particularly computational methods. This will be done through a program of software development, and through a series of retreats and workshops. The network software will be complementary to CCP13 software; together, they will eventually cover all aspects of fibre diffraction. The network emphasis on biological fibre diffraction comes from the fact that *FiberNet* is supported by the NSF Division of Molecular and Cellular Bioscience. However, fibre diffraction methods in general are usually common to biological and materials science applications, and the needs of materials scientists and others will be kept in mind, especially in software development. Of course, the network welcomes participation by all fibre diffractionists, and in the future plans to seek funding from both biologically and non-biologically oriented sources.

The experimental focus for the network will be the BioCAT X-ray beamline facility at the Advanced Photon Source synchrotron, Argonne National Laboratory. BioCAT (Biophysics Collaborative Access Team) is a national and international research resource for diffraction studies of partially ordered biological molecules, complexes of biomolecules, and cellular structures under conditions similar to those present in living cells. Many CCP13 members have collected data at the BioCAT facility. The beamline supports fibre diffraction, solution scattering, and X-ray absorption scattering, and although *FiberNet* is primarily concerned with fibre diffraction, it shares many interests with other scattering communities, and especially with small angle solution scattering. The BioCAT facilities provide a resource unique on the North American continent - worldwide, only SPring8 and ESRF operate similar facilities.

A major emphasis of the network will be cooperation between fibre diffractionists in the USA and others, particularly those in Britain. CCP13, although it is larger than *FiberNet* and more comprehensive in its scientific interests, has to some extent been a model for *FiberNet*. The director of *FiberNet* and the director of BioCAT are both co-opted members of the CCP13 Steering Committee; reciprocally (and what would a diffraction committee be without reciprocity?) the Chairman of the CCP13 Steering Committee will always be a member of the *FiberNet* Steering Committee.

The network will also be affiliated closely with the American Crystallographic Association's Fiber Diffraction Special Interest Group. The SIG is a much more loosely-organized group than CCP13, and its only activity is to organize sessions at the

Annual Meeting of the ACA. These sessions have, however, been of great value in the exchange of information among biological and synthetic fibre diffractionists in the USA. One obvious reason that the SIG has not taken more of a leading role in the co-ordination of fibre diffraction in the USA is that it has no funds of its own apart from occasional donations from industry sponsoring particular sessions; to some extent, the establishment of *FiberNet* will fill this gap. Over the years, several members of the *FiberNet* Steering Committee have served as chairs of the SIG, and like the CCP13 chairman, the SIG chair will always be a member of the *FiberNet* Steering Committee.

Like CCP13, *FiberNet* will hold annual meetings. These will be of three types, roughly rotating from year to year.

In years when the ACA SIG holds a session on biological fibre diffraction at the ACA Annual Meeting, the network will support speakers and student attendees at the session; it is hoped that this support will add new vigor to the SIG meetings.

The second type of meeting will be reminiscent of the old informal State Park meetings. Many CCP13 members will remember these meetings - the first of them, featuring Struther Arnott and Ken Holmes as keynote speakers, was held at Fall Creek Falls State Park in Tennessee in 1989, and organized by Gerald Stubbs. The second was at McCormick's Creek State Park in Indiana in 1993, organized by Rick Millane. The third, organized by Rick and Gerald, was at Jennie Wiley State Park in Kentucky (which, for those whose American geography is a bit rusty, is between Tennessee and Indiana) in 1997. These workshops were attended by about 20 to 40 participants, including speakers from the UK and Europe each time. In fact, the program for the third meeting included seven speakers from the UK and one from Italy. Some people's most vivid memory of these meetings may be Richard Denny's near-sinking of a pontoon boat at Jennie Wiley when a trailing rope caught on the bottom of the lake, but most of us also remember remarkable opportunities to exchange ideas in a relaxed atmosphere, and we are looking forward to renewing the series.

State parks are good places to exchange ideas, and with smaller and faster computers, they can even be good places to discuss and develop software. But they tend to be a bit weak in facilities for X-ray diffraction, so in some years, the meeting will be held at BioCAT. These meetings will be network retreats, like the State Park meetings, but they will feature the data collection capacity of BioCAT, and will include a strong element of experimental training. State Park and BioCAT workshops will emphasize methods rather than results; most fibre diffractionists attend other types of meeting where results dominate the presentations, but there are very few opportunities for fibre diffractionists to discuss methods. The ACA-SIG workshops may be on methods or results, depending on other themes at any given meeting.

*FiberNet* is administered by a Steering Committee, very similar in function to the CCP13 Steering Committee. At present, the members of the committee are Gerald Stubbs (Vanderbilt University, Nashville, TN, chairman), Rengaswami Chandrasekaran (Purdue University, West Lafayette, IN), Tom Irving (Illinois Institute of Technology, Chicago, IL), Dan Kirschner (Boston College, Chestnut Hill, MA), Jianpeng Ma (Baylor College of Medicine and Rice University, Houston, TX), Joseph Orgel (The Rosalind Franklin University of Medicine and Science, North Chicago, IL), and from CCP13, Trevor Forsyth (Keele and ILL), and John Squire (Imperial College London). The network has recently hired Wen Bian to develop software. Wen will be based at Vanderbilt, and will

coordinate his work with the CCP13 staff members. Wen is experienced in both software development and fibre diffraction, having worked with Chandrasekaran and Struther Arnott at Purdue University.

We are looking forward to a long and productive association between *FiberNet* and CCP13!

Gerald Stubbs - Vanderbilt University - January 2004

## US-RCN Research Assistant Profile - Wen Bian

### Dr Wen Bian

Wen Bian received his B.E. and M.A. degrees from Ocean University of China in 1994 and 1997, and his Ph.D. from Purdue University in 2001. At Purdue, he worked on the structures of industrially important polysaccharides and the relationship between structure and function in polysaccharides, using X-ray fibre diffraction analysis and computer modeling. His work at Purdue was primarily with Rengaswami Chandrasekaran, and also with Struther Arnott. While at Purdue, he developed a great interest in programming, so upon completion of his doctoral studies, he went on to complete an M.S. degree in computer science at Purdue.

Wen's software-related experience includes maintenance of in-house molecular modelling programs, development of various distributed applications, and data processing and visualization programs on Windows and UNIX platforms. He joined Gerald Stubbs's group at Vanderbilt University in January, 2004, where he will be the principal software developer for *FiberNet*, collaborating with the software developers for CCP13.

